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APPLICATION NO.	FILING DATE	FIRST NAMED INVENTOR	ATTORNEY DOCKET NO.	CONFIRMATION NO.
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Yuan-Ping Pang

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EXAMINER

NEGIN, RUSSELL SCOTT

ART UNIT

PAPER NUMBER

1631

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PAPER

Please find below and/or attached an Office communication concerning this application or proceeding.

The time period for reply, if any, is set in the attached communication.

Office Action Summary	Application No. 10/723,594	Applicant(s) PANG, YUAN-PING	
	Examiner RUSSELL S. NEGIN	Art Unit 1631	

-- The MAILING DATE of this communication appears on the cover sheet with the correspondence address --

Period for Reply

A SHORTENED STATUTORY PERIOD FOR REPLY IS SET TO EXPIRE 3 MONTH(S) OR THIRTY (30) DAYS, WHICHEVER IS LONGER, FROM THE MAILING DATE OF THIS COMMUNICATION.

- Extensions of time may be available under the provisions of 37 CFR 1.136(a). In no event, however, may a reply be timely filed after SIX (6) MONTHS from the mailing date of this communication.
- If NO period for reply is specified above, the maximum statutory period will apply and will expire SIX (6) MONTHS from the mailing date of this communication.
- Failure to reply within the set or extended period for reply will, by statute, cause the application to become ABANDONED (35 U.S.C. § 133). Any reply received by the Office later than three months after the mailing date of this communication, even if timely filed, may reduce any earned patent term adjustment. See 37 CFR 1.704(b).

Status

- 1) ☒ Responsive to communication(s) filed on 07 December 2007.
- 2a) ☐ This action is **FINAL**. 2b) ☒ This action is non-final.
- 3) ☐ Since this application is in condition for allowance except for formal matters, prosecution as to the merits is closed in accordance with the practice under *Ex parte Quayle*, 1935 C.D. 11, 453 O.G. 213.

Disposition of Claims

- 4) ☒ Claim(s) 37-72 is/are pending in the application.
- 4a) Of the above claim(s) _____ is/are withdrawn from consideration.
- 5) ☐ Claim(s) _____ is/are allowed.
- 6) ☒ Claim(s) 37-72 is/are rejected.
- 7) ☐ Claim(s) _____ is/are objected to.
- 8) ☐ Claim(s) _____ are subject to restriction and/or election requirement.

Application Papers

- 9) ☐ The specification is objected to by the Examiner.
- 10) ☒ The drawing(s) filed on 09 April 2004 is/are: a) ☒ accepted or b) ☐ objected to by the Examiner.
Applicant may not request that any objection to the drawing(s) be held in abeyance. See 37 CFR 1.85(a).
Replacement drawing sheet(s) including the correction is required if the drawing(s) is objected to. See 37 CFR 1.121(d).
- 11) ☐ The oath or declaration is objected to by the Examiner. Note the attached Office Action or form PTO-152.

Priority under 35 U.S.C. § 119

- 12) ☐ Acknowledgment is made of a claim for foreign priority under 35 U.S.C. § 119(a)-(d) or (f).
- a) ☐ All b) ☐ Some * c) ☐ None of:
1. ☐ Certified copies of the priority documents have been received.
2. ☐ Certified copies of the priority documents have been received in Application No. _____.
3. ☐ Copies of the certified copies of the priority documents have been received in this National Stage application from the International Bureau (PCT Rule 17.2(a)).

* See the attached detailed Office action for a list of the certified copies not received.

Attachment(s)

- | | |
|--|---|
| 1) <input checked="" type="checkbox"/> Notice of References Cited (PTO-892) | 4) <input type="checkbox"/> Interview Summary (PTO-413) |
| 2) <input type="checkbox"/> Notice of Draftsperson's Patent Drawing Review (PTO-948) | Paper No(s)/Mail Date. _____ |
| 3) <input type="checkbox"/> Information Disclosure Statement(s) (PTO/SB/08) | 5) <input type="checkbox"/> Notice of Informal Patent Application |
| Paper No(s)/Mail Date _____ | 6) <input type="checkbox"/> Other: _____ |

DETAILED ACTION

Comments

Applicants' amendments and request for reconsideration in the communication filed on 7 December 2007 are acknowledged and the amendments are entered.

Claims 37-72 are pending and examined in the instant application.

Withdrawn Rejections

The rejections of claims 37-54 under 35 U.S.C. 101 because the claimed invention is directed to non-statutory subject matter are withdrawn in view of amendments filed on 7 December 2007.

The rejections of claims 37-72 under 35 U.S.C. 112, second paragraph, as being indefinite for failing to particularly point out and distinctly claim the subject matter which applicant regards as the invention are withdrawn in view of amendments filed on 7 December 2007.

Claim Rejections - 35 USC § 101

The following rejection is reiterated from the previous Office action:

35 U.S.C. 101 reads as follows:

Whoever invents or discovers any new and useful process, machine, manufacture, or composition of matter, or any new and useful improvement thereof, may obtain a patent therefor, subject to the conditions and requirements of this title.

Claims 55-72 are rejected under 35 U.S.C. 101 because the claimed invention is directed to non-statutory subject matter.

Claim 55 is drawn to a computer readable medium having computer executable instructions stored thereon to execute a simulation. Since the specification is silent on what constitutes "computer readable media," this claim can be interpreted broadly such that this "computer readable media" encompasses carrier waves which, per se, are not statutory. Consequently, an embodiment of claims 55-72 reads on a carrier wave resulting in a set of claims that is not statutory. See MPEP 2106.

Response to Arguments:

Applicant's arguments filed 7 December 2007 have been fully considered but they are not persuasive.

Applicant argues that the amendment "for observation by a user on a display" results in a statutory claim because the output of the claim is now useful, concrete, and tangible. This argument is not persuasive because, as discussed above, an embodiment of the instant claim still reads on non-statutory material (i.e. carrier waves). If a single embodiment of a claim reads on nonstatutory subject matter, the entire claim is rejected as not statutory.

Claim Rejections - 35 USC § 112

The following rejection is NEWLY applied:

SCOPE OF ENABLEMENT

The following is a quotation of the first paragraph of 35 U.S.C. 112:

The specification shall contain a written description of the invention, and of the manner and process of making and using it, in such full, clear, concise, and exact terms as to enable any person skilled in the

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art to which it pertains, or with which it is most nearly connected, to make and use the same and shall set forth the best mode contemplated by the inventor of carrying out his invention.

Claims 37-72 rejected under 35 U.S.C. 112, first paragraph, because while the claims recite that "said center atom is covalently linked to said one or more dummy atoms," the specification defines "dummy atoms" as having van der Waals radii of at or about zero (see below). The specification does not enable any person skilled in the art to which it pertains, or with which it is most nearly connected, to make and/or use the invention commensurate in scope with these claims, when there is a covalent bond between the center atom (with a non-zero radius) with these dummy atoms (in the instance where each dummy atom has a radius of zero).

In *In re Wands* (8 USPQ2d 1400 (CAFC 1988)) the CAFC considered the issue of enablement in molecular biology. The CAFC summarized eight factors to be considered in a determination of "undue experimentation." These factors include: (a) the quantity of experimentation necessary; (b) the amount of direction or guidance presented; (c) the presence or absence of working examples; (d) the nature of the invention; (e) the state of the prior art; (f) the relative skill of those in the art; (g) the predictability of the art; and (h) the breadth of the claims.

In considering the factors for the instant claims:

a) In order to use the claimed invention one of skill in the art may use a dummy atom with a radius of zero for covalent bonding. While the claims are enabled for dummy atoms with "non-zero" radii, for the reasons discussed below, there would be an unpredictable amount of experimentation required to practice the claimed invention.

b) The specifications discloses the following commentary about dummy atoms on

page 3, lines 11-12 and lines 25-30:

...the dummy atoms may have no van der Waals interaction with other atoms, i.e. $r^*=0$ & $e=0$...

A simulated metal ion molecule for use in a molecular dynamics simulation includes a center atom having a van der Waals radius greater than zero covalently linked to one or more dummy atoms having a van der Waals radius of about zero...

Consequently, the specification discloses that dummy atoms can have a radius of zero, yet still be covalently bonded to other atoms.

c) The specification provides working examples of identification of simulating a single and two tetrahedral zinc molecules. However, while the specification gives radii of the entire zinc molecule (i.e. see page 20, line 7); the examples are silent on radii of actual “dummy atoms” used in the exemplary simulations.

d) The nature of the invention, simulation of metal ions, in complex.

e) The prior art does not show covalent bonding of an atom to another atom having a radius of zero. In fact, Zumdahl [Chemistry, 1986, pages 42-44 and 279-280], defines covalent bonds as atoms forming bonds by sharing electrons. Figures 2.16-2.18 on pages 43-44 of Zumdahl illustrate molecules with covalent bonds in which each atom has a radius greater than zero. Additionally, Figure 7.35 and pages 279-280 shows that atoms have a non-zero radius. In other words, to form a covalent bond, electrons must be shared between the two atoms in the chemical bond. For electrons to be shared between two atoms, each of the atoms in the bond must have a non-zero radius.

f) The skill of those in the art of simulating metal ions is high.

g) The predictability of the relationship of a covalent bond between two atoms in which one of the atoms has a radius of zero is not known in the prior art.

h) The claims are broad in that they encompass (in light of the specification) covalent bonding to "dummy atoms" having a radius of anywhere between zero and "about zero," in which "about zero" is not defined in the instant specification.

The skilled practitioner would first turn to the instant description for guidance in using the claimed invention. However, the description lacks clear evidence on how to form a covalent bond with a dummy atom having a radius of zero. As such, the skilled practitioner would turn to the prior art for such guidance, however the prior art does not discuss covalent bonds with atoms with radii of zero. Finally, said practitioner would turn to trial and error experimentation to determine how to form a covalent bond with an atom with a radius of zero. Such amounts to undue experimentation.

Response to Arguments

Applicant's additional arguments with respect to claims 37-72 have been considered but are moot in view of the new ground(s) of rejection.

Conclusion

No claim is allowed.

Papers related to this application may be submitted to Technical Center 1600 by facsimile transmission. Papers should be faxed to Technical Center 1600 via the central PTO Fax Center. The faxing of such pages must conform with the notices published in the Official Gazette, 1096 OG 30 (November 15, 1988), 1156 OG 61

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(November 16, 1993), and 1157 OG 94 (December 28, 1993)(See 37 CFR § 1.6(d)).

The Central PTO Fax Center Number is (571) 273-8300.

Any inquiry concerning this communication or earlier communications from the examiner should be directed to Russell Negin, Ph.D., whose telephone number is (571) 272-1083. The examiner can normally be reached on Monday-Friday from 7am to 4pm.

If attempts to reach the examiner by telephone are unsuccessful, the examiner's Supervisor, Marjorie Moran, Supervisory Patent Examiner, can be reached at (571) 272-0720.

Information regarding the status of the application may be obtained from the Patent Application Information Retrieval (PAIR) system. Status information for published applications may be obtained from either Private PAIR or Public PAIR. Status information for unpublished applications is available through Private PAIR only. For more information on the PAIR system, contact the Electronic Business Center (EBC) at 866-217-9197 (toll-free).

/RSN/
2 March 2008

/Marjorie Moran/
Supervisory Patent Examiner, Art Unit 1631